Pyridine, 3-ethyl-4-methyl-

Other names:	3-Ethyl-4-methylpyridine
	3-Ethyl-4-picoline
	3-Ethyl-«gamma»-picoline
	3-Ethyl-Â«gammaÂ»-picoline
	4-Methyl-3-ethylpyridine
	4-Picoline, 3-ethyl-
	NSC 62016
	«beta»-Collidine
	«beta»-Ethyl-«gamma»-methylpyridine
	«beta»-Ethyl-«gamma»-picoline
	Â«betaÂ»-Collidine
	Â«betaÂ»-Ethyl-Â«gammaÂ»-methylpyridine
	Â«betaÂ»-Ethyl-Â«gammaÂ»-picoline
Inchi:	InChI=1S/C8H11N/c1-3-8-6-9-5-4-7(8)2/h4-6H,3H2,1-2H3
InchiKey:	JDQNYWYMNFRKNQ-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1cnccc1C
Mol. weight [g/mol]:	121.18
CAS:	529-21-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.952		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
rinpol	1011.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1545.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64809e+01
Coeff. B	-4.53073e+03
Coeff. C	-7.21300e+01
Temperature range (K), min.	351.92
Temperature range (K), max.	477.77

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C529215&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure